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Physics 704 **HOMEWORK ASSIGNMENT #1** Spring 2006

1. LMB, problem 3.8.4 A.

2. For the interface between a *solid* and a liquid or gas, α is not simply the line tension (generalization to 1+1 dimensions of surface tension σ in 2+1 dimensions, as in PB eqn. 4.72) becomes a function of interface direction. For simplicity, continue as in the previous problem to assume a 1+1 dimensional model, with the interface at $z(x)$. Let $\sigma \rightarrow \sigma(\theta)$, where θ = arctan (dz/dx). Show that for small distortions, σ is replaced by what is called the stiffness or rigidity, given by $\sigma(0) + d^2\sigma/d\theta^2|_{\theta=0}$. Hint: consider a small line segment making an angle θ with respect to the flat interface. The increase in energy compared to the flat segment is due to both the increase in $\sigma(\theta)$ relative to $\sigma(0)$ and to the increase in length of the line segment (i.e. the hypotenuse of a right triangle). Expand in θ, keeping the leading terms. Note that since $\theta = 0$ is the stable direction, $d\sigma/d\theta|_{\theta=0} = 0$.

3. We did most of LMB 3.8.7. Do a) part 5 iii and b) part 6. If you are not fluent in any package like Mathematica, you may substitute 5 i and ii.

4. Consider LMB, problem 3.8.8. First understand the equations in part 5. Then do parts 6 and 8.

5. Consider a simple cubic lattice with lattice constant a. For full symmetry, we can consider a slab that is n layers thick, with periodic boundary conditions in the 2 in-plane (x-y) directions. In that plane, the cell need only contain a single atom.
a) Argue that the energy of this construction in an electronic structure calculation is

$$nE_B + 2E_S$$

where E_B is the bulk energy per atomic volume and E_S is the surface energy per atomic area.
b) If another "layer" is added (so another atom), what is the total energy?
c) Use this information to indicate how to separate out E_B and E_S when computing the energy of a slab.